

\* \* \* \* \* \* \* \* \* Welcome to STN International \* \* \* \* \*

<u>NEWS 1</u>	Web Page URLs for STN Seminar Schedule - N. America
<u>NEWS 2</u>	"Ask CAS" for self-help around the clock
<u>NEWS 3</u> May 12	EXTEND option available in structure searching
<u>NEWS 4</u> May 12	Polymer links for the POLYLINK command completed in REGISTRY
<u>NEWS 5</u> May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
<u>NEWS 6</u> May 27	CAplus super roles and document types searchable in REGISTRY
<u>NEWS 7</u> Jun 28	Additional enzyme-catalyzed reactions added to CASREACT
<u>NEWS 8</u> Jun 28	ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R)
<u>NEWS 9</u> Jul 12	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
<u>NEWS 10</u> Jul 30	BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
<u>NEWS 11</u> AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
<u>NEWS 12</u> AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
<u>NEWS 13</u> AUG 02	STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
<u>NEWS 14</u> AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
<u>NEWS 15</u> AUG 04	Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004

<u>NEWS EXPRESS</u>	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
<u>NEWS HOURS</u>	STN Operating Hours Plus Help Desk Availability
<u>NEWS INTER</u>	General Internet Information
<u>NEWS LOGIN</u>	Welcome Banner and News Items
<u>NEWS PHONE</u>	Direct Dial and Telecommunication Network Access to STN
<u>NEWS WWW</u>	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* \* \* \* \* STN Columbus \* \* \* \* \* \* \* \* \* \* \*

FILE 'HOME' ENTERED AT 10:54:43 ON 09 AUG 2004

=> file reg	COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST		0.21	0.21

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 09 AUG 2004  
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Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 7 AUG 2004 HIGHEST RN 723734-66-5  
DICTIONARY FILE UPDATES: 7 AUG 2004 HIGHEST RN 723734-66-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:

<http://www.cas.org/ONLINE/DBSS/registryss.html>

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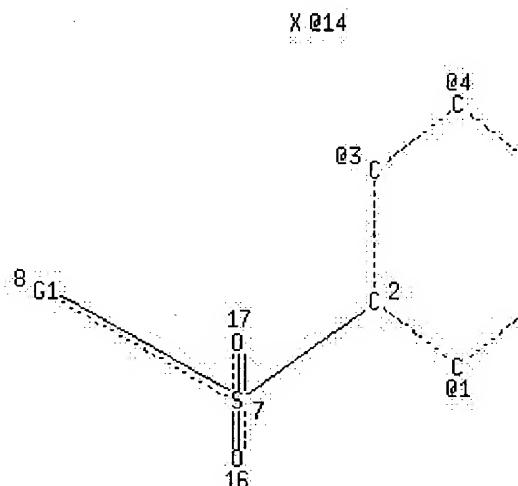
L1        STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1            STR

AK19N M2

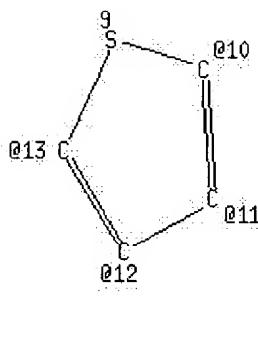


Page 1-A

h       eb c      g cg b      cg

eb

C4 @15 :



Page 1-B

VAR G1=18/19

VPA 14-1/3/4/5/6 S

VPA 15-10/11/12/13 S

## NODE ATTRIBUTES:

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HCOUNT IS M2      AT  19
NSPEC  IS R       AT   1
NSPEC  IS R       AT   2
NSPEC  IS R       AT   3
NSPEC  IS R       AT   4
NSPEC  IS R       AT   5
NSPEC  IS R       AT   6
NSPEC  IS C       AT   7
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NSPEC  IS R       AT  10
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NSPEC  IS C       AT  17

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DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 7 14 16 17 18 19

DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE

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SAMPLE SEARCH INITIATED 10:57:09 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 1647 TO ITERATE

60.7% PROCESSED 1000 ITERATIONS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

2 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 30506 TO 35374

h eb c g cg b cg

eb

PROJECTED ANSWERS: 2 TO 173

L2 2 SEA SSS SAM L1

=> s 11 full  
 THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS  
 DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
 FULL SEARCH INITIATED 10:57:12 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 32122 TO ITERATE

100.0% PROCESSED 32122 ITERATIONS 41 ANSWERS  
 SEARCH TIME: 00.00.01

L3 41 SEA SSS FUL L1

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 ENTRY SESSION  
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FILE 'HCPLUS' ENTERED AT 10:57:16 ON 09 AUG 2004  
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FILE COVERS 1907 - 9 Aug 2004 VOL 141 ISS 7  
 FILE LAST UPDATED: 8 Aug 2004 (20040808/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 13  
 L4 14 L3

=> s 14 and brown, d?/au  
 7837 BROWN, D?/AU  
 L5 2 L4 AND BROWN, D?/AU

=> d 15, ibib abs fhitstr, 1-2

L5 ANSWER 1 OF 2 HCPLUS COPYRIGHT 2004 ACS on STN

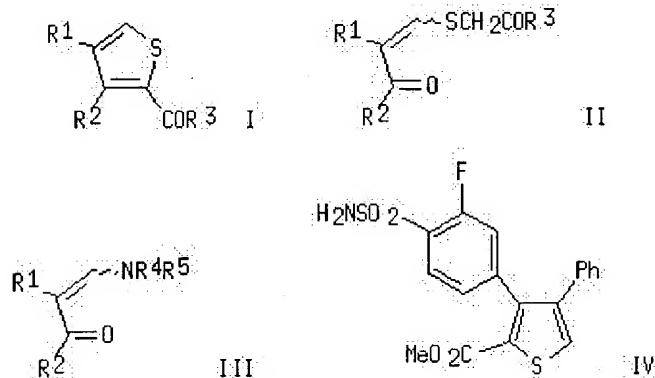
Full	Search
Text	References

ACCESSION NUMBER: 2001:798214 HCPLUS  
 DOCUMENT NUMBER: 135:344368  
 TITLE: Process for the regioselective synthesis of 3,4-diaryl substituted thiophenes  
 INVENTOR(S): Brown, David L.; Ludwig, Cindy L.

PATENT ASSIGNEE(S): Pharmacia Corporation, USA  
 SOURCE: PCT Int. Appl., 74 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2001081333</u>	A2	20011101	<u>WO 2001-US13092</u>	20010420
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
<u>US 2002183362</u>	A1	20021205	<u>US 2001-839424</u>	20010420
<u>EP 1276736</u>	A2	20030122	<u>EP 2001-928781</u>	20010420
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
<u>US 6600052</u>	B1	20030729	<u>US 2001-838986</u>	20010420
<u>JP 2003531202</u>	T2	20031021	<u>JP 2001-578424</u>	20010420
<u>US 2003232996</u>	A1	20031218	<u>US 2003-258507</u>	20030416
<u>PRIORITY APPLN. INFO.:</u>			<u>US 2000-199533P</u>	P 20000425
			<u>US 2000-253380P</u>	P 20001127
			<u>WO 2001-US13092</u>	W 20010420

OTHER SOURCE(S): CASREACT 135:344368; MARPAT 135:344368  
 GI



AB A novel process for the regioselective prepn. of I, via the intermediates II and III using an alkali metal alkoxide ring cyclizing reagent where (R1 and R2 = substituted carbocycle or heterocycle; R3 = OR6 or NR7R8 and R6, R7 and R8 = H, (un)heterosubstituted hydrocarbyl; R4 and R5 are independently H and optionally substituted alkyl), was accomplished. Thus IV was prepnd. in 66 % yield via the enamine intermediate of Me 3-[3-fluoro-4-(methylthio)phenyl]-4-phenyl-2-thiophencarboxylate.

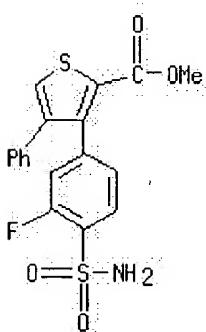
IT 370874-59-2P  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of 3,4-diarylthiophene)

RN 370874-59-2 HCAPLUS

h eb c g cg b cg

eb

CN 2-Thiophenecarboxylic acid, 3-[4-(aminosulfonyl)-3-fluorophenyl]-4-phenyl-, methyl ester (9CI) (CA INDEX NAME)

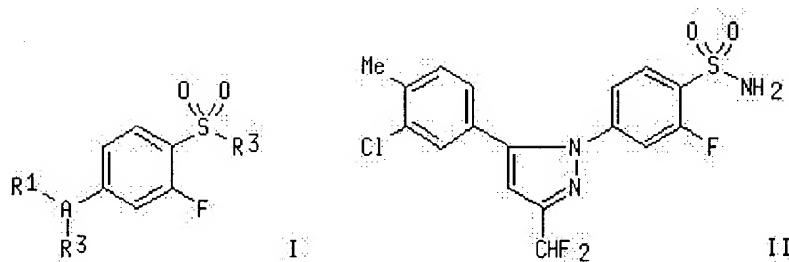


L5 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  Summary  
 Text  References

ACCESSION NUMBER: 2001:798213 HCAPLUS  
 DOCUMENT NUMBER: 135:344477  
 TITLE: Preparation of 2-fluorobenzenesulfonyl-heterocycles with COX-1 and COX-2 inhibiting activity for pharmaceutical use in the treatment of inflammation  
 INVENTOR(S): Brown, David L.; Graneto, Matthew J.; Ludwig, Cindy L.; Talley, John J.  
 PATENT ASSIGNEE(S): Pharmacia Corporation, USA  
 SOURCE: PCT Int. Appl., 242 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001081332	A2	20011101	WO 2001-US12983	20010420
WO 2001081332	A3	20020404		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002183362	A1	20021205	US 2001-839424	20010420
EP 1296971	A2	20030402	EP 2001-927279	20010420
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
US 6600052	B1	20030729	US 2001-838986	20010420
JP 2003531201	T2	20031021	JP 2001-578423	20010420
US 2004092552	A1	20040513	US 2003-258493	20030711
<u>PRIORITY APPLN. INFO.:</u>			US 2000-199533P	P 20000425
			US 2000-253380P	P 20001127
			WO 2001-US12983	W 20010420
OTHER SOURCE(S): MARPAT 135:344477				
GI				



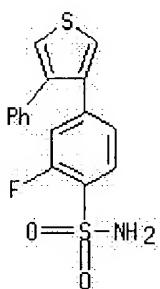
AB 2-Fluorobenzenesulfonyl-heterocycles, such as I [A = 5 or 6 membered heterocycle or carbocycle, such as pyrazole, thiophene, isoxazole, furan; R1 = cyclohexyl, pyridinyl, Ph; R2 = Me, NH<sub>2</sub>; R3 = H, oxo, CN, halogen, alkyl, alkenyl, carboxyl, haloalkyl, heterocyclyl, cycloalkenyl, aminocarbonyl, etc.] with COX-1 and COX-2 inhibiting activity, were prep'd. for therapeutic use as anti-inflammatory agents. Thus, pyrazole II was prep'd. via a multistep synthetic sequence in which the last step was a cyclocondensation reaction of 4-H<sub>2</sub>NSO<sub>2</sub>-3-F-C<sub>6</sub>H<sub>3</sub>NHNH<sub>2</sub> and 3-Cl-4-Me-C<sub>6</sub>H<sub>3</sub>COCH<sub>2</sub>COCHF<sub>2</sub> achieved by refluxing for 1 h. concd. HCl in EtOH to give II with 53% yield. The prep'd. heterocycles were tested for COX-1 and -2 inhibiting activity.

IT 370874-28-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of 2-fluorobenzenesulfonyl-heterocycles with COX-1 and COX-2 inhibiting activity for pharmaceutical use in the treatment of inflammation)

RN 370874-28-5 HCAPLUS

CN Benzenesulfonamide, 2-fluoro-4-(4-phenyl-3-thienyl)- (9CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 10:54:43 ON 09 AUG 2004)

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 09 AUG 2004

L1   STRUCTURE UPLOADED

L2   2 S L1

L3   41 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 10:57:16 ON 09 AUG 2004

L4   14 S L3

L5   2 S L4 AND BROWN, D?/AU

=> s 14 not 15

h

eb c

g cg b

cg

eb

L6 12 L4 NOT L5

=> s 16 and graneto, m?/au  
 40 GRANETO, M?/AU  
 L7 0 L6 AND GRANETO, M?/AU

=> s 16 and ludwig, c?/au  
 270 LUDWIG, C?/AU  
 L8 0 L6 AND LUDWIG, C?/AU

=> d 16, ibib abs fhitstr, 1~12

L6 ANSWER 1 OF 12 HCPLUS COPYRIGHT 2004 ACS on STN

**Full** **Search**  
**Text** **References**

ACCESSION NUMBER: 2004:565073 HCPLUS  
 TITLE: Use of cathepsin k inhibitors for the treatment of glaucoma  
 INVENTOR(S): Shepard, Allan; Clark, Abbot F.; Jacobson, Nasreen  
 PATENT ASSIGNEE(S): Alcon, Inc., Switz.  
 SOURCE: PCT Int. Appl., 57 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2004058238</u>	A1	20040715	<u>WO 2003-US40511</u>	20031219
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: US 2002-436126P P 20021223  
 AB Compns. contg. inhibitors of cathepsin K (CTSK) expression and/or activity are provided. Methods for the treatment of glaucoma using the compns. of the invention are further provided. The cathepsin K antagonist is selected from, but not limited to, the group consisting of monensin, brefeldin A, tunicamycin and 1,3-bis(acylamino)-2-propanone derivs., cycloaltilisin 6, cycloaltilisin 7, AC-3-1, AC-3-3, AC-5-1, haploscleridamine, SB-331750, SB-357114, peptidomimetic aminomethyl ketones,  $\alpha,\alpha'$ -diacylamino ketones, alkoxyethyl ketones, cyanamides, pyridoxal propionate derivs. (including Clik-164 and Clik-166), SB-290190,  $\alpha$ -alkoxy ketone derivs., cyanamide derivs., and  $\text{Na-acyl-}\alpha\text{-amino acid-(arylaminoethyl)amides.}$

IT 190658-17-4

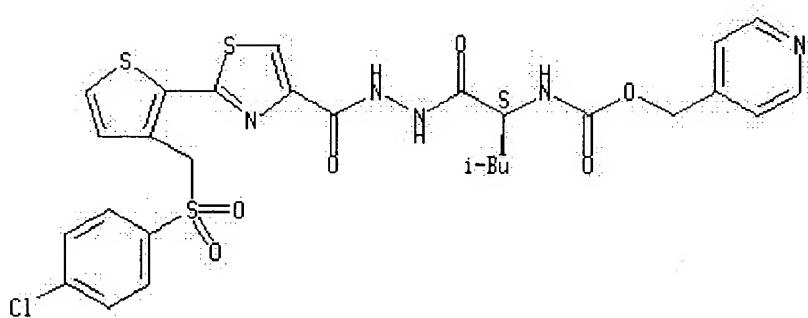
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (use of cathepsin k inhibitors for treatment of glaucoma)

RN 190658-17-4 HCPLUS

CN 4-Thiazolecarboxylic acid, 2-[3-[(4-chlorophenyl)sulfonyl]methyl]-2-

thienyl]-, 2-[(2S)-4-methyl-1-oxo-2-[(4-pyridinylmethoxy)carbonyl]amino]pentyl]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L6 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

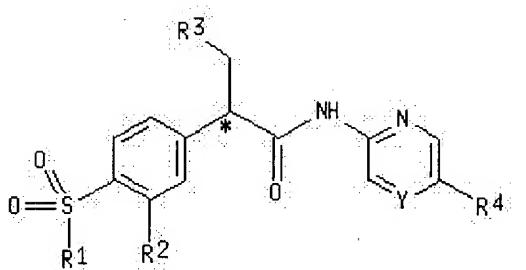
Full  Citation  
 Text  References

ACCESSION NUMBER: 2004:515493 HCAPLUS  
 DOCUMENT NUMBER: 141:71565  
 TITLE: Preparation of pyrazines and related compounds as glucokinase activators for the treatment of type II diabetes  
 INVENTOR(S): Chen, Shaoqing; Corbett, Wendy Lea; Guertin, Kevin Richard; Haynes, Nancy-Ellen; Kester, Robert Francis; Mennona, Francis A.; Mischke, Steven Gregory; Qian, Yimin; Sarabu, Ramakanth; Scott, Nathan Robert; Thakkar, Kshitij Chhabilbhai  
 PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.  
 SOURCE: PCT Int. Appl., 243 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2004052869</u>	A1	20040624	<u>WO 2003-EP14055</u>	20031211
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<u>US 2004147748</u>	A1	20040729	<u>US 2003-732838</u>	20031210
<u>PRIORITY APPLN. INFO.:</u>			<u>US 2002-432806P</u>	P 20021212
			<u>US 2003-524531P</u>	P 20031124

GI



AB Title compd. I [R1 = alkyl; R2 = H, halo, nitro, etc.; R3 = cycloalkyl; R4 = SO<sub>2</sub>NR<sub>5</sub>R<sub>6</sub>, NHSO<sub>2</sub>CH<sub>3</sub>, [CH<sub>2</sub>]<sub>m</sub>NMe<sub>2</sub>, etc.; R5 = H, alkyl; R6 = alkyl; Y = CH, N; \* denotes an asym. carbon] and their pharmaceutically acceptable salts were prep'd. For example, the Pd-catalyzed coupling of 2-amino-5-bromopyrazine with NaSMe, followed by reaction with (2R)-(3-chloro-4-methanesulfonylphenyl)-3-cyclopentylpropionic acid afforded compd. (R)-I [R1 = Me; R2 = Cl; R3 = cyclopetyl; R4 = SMe; Y = N] in 22.1% overall yield. In glucokinase activity assays (in vitro) using glucose-6-phosphate dehydrogenase (G6PDH), compds. I exhibited SC1.5 values less than or equal to 100 μM. Formulations are given. Compds. I are claimed useful for the treatment and prophylaxis of II type diabetes.

IT 710321-98-5P

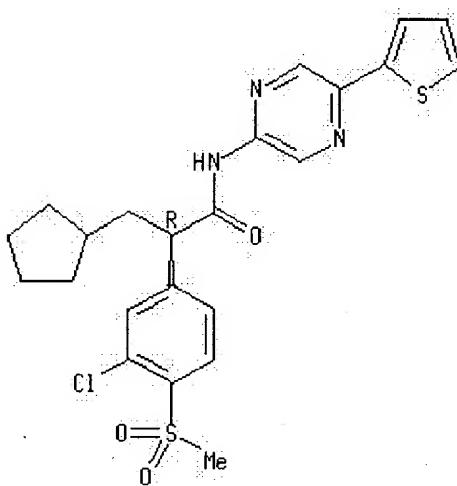
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of pyrazines and related compds. as glucokinase activators for the treatment of type II diabetes)

RN 710321-98-5 HCAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



L6 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text  Citations  Structure  Reactions

ACCESSION NUMBER:

2002:145039 HCAPLUS

DOCUMENT NUMBER:

136:325469

TITLE:

4-(4-Cycloalkyl/aryl-oxazol-5-yl)benzenesulfonamides as Selective Cyclooxygenase-2 Inhibitors: Enhancement of the Selectivity by Introduction of a Fluorine Atom and Identification of a Potent, Highly Selective, and

AUTHOR(S): Orally Active COX-2 Inhibitor JTE-522  
 Hashimoto, Hiromasa; Imamura, Katsuaki; Haruta,  
 Jun-ichi; Wakitani, Korekiyo

CORPORATE SOURCE: Central Pharmaceutical Research Institute, JT Inc.,  
 Takatsuki, Osaka, 569-1125, Japan

SOURCE: Journal of Medicinal Chemistry (2002), 45(7),  
 1511-1517

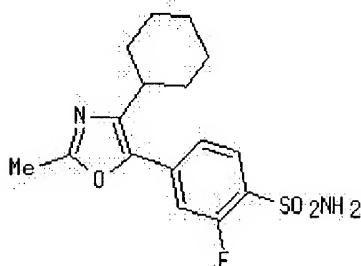
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

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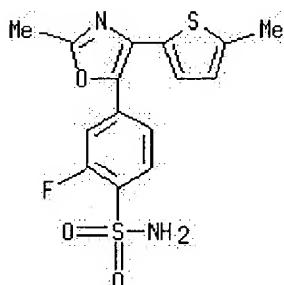
AB A series of 4-(4-cycloalkyl/aryl-oxazol-5-yl)benzenesulfonamide derivs., e.g., I, were synthesized and evaluated for their abilities to inhibit cyclooxygenase-2 (COX-2) and cyclooxygenase-1 (COX-1) enzymes. In this series, substituent effects at the ortho position to the sulfonamide group on the Ph ring were examd. Most substituents reduced or lost both COX-2 and COX-1 activities. In contrast, introduction of a fluorine atom preserved COX-2 potency and notably increased COX1/COX-2 selectivity. This work led to the identification of a potent, highly selective, and orally active COX-2 inhibitor I (JTE-522), which is currently in phase II clin. trials for the treatment of rheumatoid arthritis, osteoarthritis, and acute pain.

IT 415679-14-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
 (prepn. of substituted benzenesulfonamides as selective cyclooxygenase-2 inhibitors from substituted benzyl bromides via coupling with acid chloride, conversion to  $\alpha$ -acetoxy ketones, cyclocondensation to form oxazoles and sulfonamidation)

RN 415679-14-0 HCPLUS

CN Benzenesulfonamide, 2-fluoro-4-[2-methyl-4-(5-methyl-2-thienyl)-5-oxazolyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

26

THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 12 HCPLUS COPYRIGHT 2004 ACS on STN

Full Text  Abstract  References

ACCESSION NUMBER: 2002:72091 HCPLUS  
 DOCUMENT NUMBER: 136:134566  
 TITLE: Synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compounds as  $\beta_3$ -adrenergic agonists  
 INVENTOR(S): Evers, Britta; Jesudason, Cynthia Darshini; Karanjawala, Rushad Eruch; Remick, David Michael; Ruehter, Gerd; Sall, Daniel Jon; Schotten, Theo; Siegel, Miles Goodman; Stenzel, Wolfgang; Stucky, Russell Dean; Werner, John Arnold  
 PATENT ASSIGNEE(S): Eli Lilly and Company, USA  
 SOURCE: PCT Int. Appl., 96 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 2002006276</u>	A1	20020124	<u>WO 2001-US16519</u>	20010709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
<u>AU 2001072917</u>	A5	20020130	<u>AU 2001-72917</u>	20010709
<u>EP 1303509</u>	A1	20030423	<u>EP 2001-952125</u>	20010709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
<u>BR 2001012409</u>	A	20030722	<u>BR 2001-12409</u>	20010709
<u>JP 2004504320</u>	T2	20040212	<u>JP 2002-512179</u>	20010709
<u>US 2003191156</u>	A1	20031009	<u>US 2002-311112</u>	20021213
<u>US 6730792</u>	B2	20040504		
<u>NO 2003000098</u>	A	20030109	<u>NO 2003-98</u>	20030109
<u>HR 2003000018</u>	A1	20030430	<u>HR 2003-18</u>	20030113
<u>PRIORITY APPLN. INFO.:</u>				
			<u>US 2000-217965P</u>	P 20000713
			<u>US 2000-241614P</u>	P 20001019
			<u>US 2001-292988P</u>	P 20010523
			<u>WO 2001-US16519</u>	W 20010709

OTHER SOURCE(S): MARPAT 136:134566

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [A1-3 = C, N provided that only one of A1-3 can be nitrogen; Het = (un)substituted, optionally benzofused 5 or 6 membered heterocyclic ring; R1,1a,1b = H, halo, OH, alkyl, alkoxy, haloalkyl, SO<sub>2</sub>-alkyl; R2 = H, alkyl; R3 = H alkyl; R4 = H, alkyl; or R3 and R4

combine with the carbon to which both are attached to form a C3-C6 cyclic ring; or R4 and X1 combine with the carbon to which both are attached to form a C3-C8 cyclic ring; or R4 combines with X1, the carbon to which both are attached, and the Ph group to which X1 is attached to form a benzofused cycloalkyl radical; X is OCH<sub>2</sub>, SCH<sub>2</sub>, bond; X1 = bond, divalent hydrocarbon moiety; X2 = O, S, NH, NHSO<sub>2</sub>, SO<sub>2</sub>NH, CH<sub>2</sub>, bond; X3 = (un)substituted Ph, 5 or 6 membered heterocyclic ring] were prep'd. For instance, 2-(1-methylpyrazol-3-yl)phenol was reacted with (2S)-glycidyl 3-nitrobenzenesulfonate (THF, t-BuOK, reflux, 16 h) to give epoxide II. This was reacted with the amine derived from 4-(2-amino-2-methylpropyl)phenol and 2-chloro-3-cyanopyridine (alc. solvent, 80°C, 2-72 h) to give III. The intrinsic activity (Emax) of representative compds. of the invention was assessed relative to isoproterenol (a nonselective β3-agonist); III had Emax = 55.0%. I are used in the treatment of diabetes, obesity, etc.

IT 391922-26-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as β3-adrenergic agonists)

RN 391922-26-2 HCAPLUS

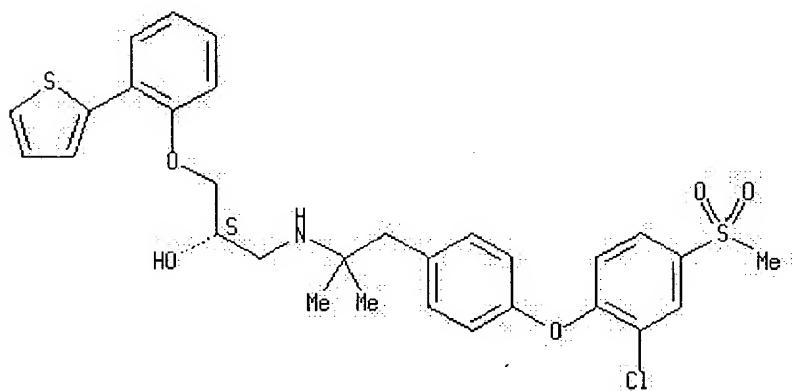
CN 2-Propanol, 1-[[2-[4-[2-chloro-4-(methylsulfonyl)phenoxy]phenyl]-1,1-dimethylethyl]amino]-3-[2-(2-thienyl)phenoxy]-, (2S)-, trifluoroacetate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 391922-25-1

CMF C30 H32 Cl N O5 S2

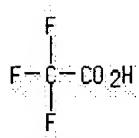
Absolute stereochemistry.



CM 2

CRN 76-05-1

CMF C2 H F3 O2



REFERENCE COUNT:

13

THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS

h

eb c g cg b cg

eb

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text	Abstract
	References

ACCESSION NUMBER: 2000:637744 HCAPLUS  
 DOCUMENT NUMBER: 134:39080  
 TITLE: A method for including protein flexibility in protein-ligand docking: improving tools for database mining and virtual screening  
 AUTHOR(S): Broughton, H. B.  
 CORPORATE SOURCE: Merck, Sharp & Dohme Neuroscience Research Centre, Essex, UK  
 SOURCE: Journal of Molecular Graphics & Modelling (2000), 18 (3), 247-257  
 CODEN: JMGMFI; ISSN: 1093-3263  
 PUBLISHER: Elsevier Science Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Second-generation methods for docking ligands into their biol. receptors, such as FLOG, provide for flexibility of the ligand but not of the receptor. Mol. dynamics based methods, such as free energy perturbation, account for flexibility, solvent effects, etc., but are very time consuming. We combined the use of statistical anal. of conformational samples from short-run protein mol. dynamics with grid-based docking protocols and demonstrated improved performance in two test cases. Our statistical anal. explores the importance of the av. strength of a potential interaction with the biol. target and optionally applies a weighting depending on the variability in the strength of the interaction seen during dynamics simulation. Using these methods, we improved the no. of known dihydrofolate reductase ligands found in the top-ranked 10% of a database of drug-like mols., in searches based on the three-dimensional structure of the protein. These methods are able to match the ability of manual docking to assess likely inactivity on steric grounds and indeed to rank order ligands from a homologous series of cyclooxygenase-2 inhibitors with good correlation to their true activity. Furthermore, these methods reduce the need for human intervention in setting up mol. docking expts.

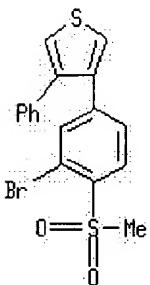
IT 312611-71-5

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)

(method for including protein flexibility in protein-ligand docking - improving tools for database mining and virtual screening)

RN 312611-71-5 HCAPLUS

CN Thiophene, 3-[3-bromo-4-(methylsulfonyl)phenyl]-4-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

32

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 12 HCPLUS COPYRIGHT 2004 ACS on STN

Full Text	References
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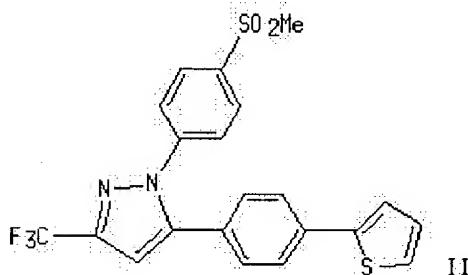
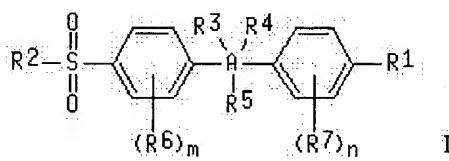
ACCESSION NUMBER: 1999:795808 HCPLUS  
 DOCUMENT NUMBER: 132:35714  
 TITLE: Preparation of heterocycll sulfonylbenzene compounds as anti-inflammatory/analgesic agents.  
 INVENTOR(S): Ando, Kazuo; Kato, Tomoki; Kawai, Akiyoshi; Nonomura, Tomomi  
 PATENT ASSIGNEE(S): Pfizer Pharmaceuticals Inc., USA  
 SOURCE: PCT Int. Appl., 236 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 9964415</u>	A1	19991216	<u>WO 1999-IB970</u>	19990531
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
<u>AU 9938414</u>	A1	19991230	<u>AU 1999-38414</u>	19990531
<u>EP 1086097</u>	A1	20010328	<u>EP 1999-921043</u>	19990531
<u>EP 1086097</u>	B1	20040519		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
<u>JP 2002517496</u>	T2	20020618	<u>JP 2000-553424</u>	19990531
<u>AT 267196</u>	E	20040615	<u>AT 1999-921043</u>	19990531
<u>ZA 9903897</u>	A	20010104	<u>ZA 1999-3897</u>	19990610
<u>US 6294558</u>	B1	20010925	<u>US 1999-446049</u>	19991215
<u>US 2002045654</u>	A1	20020418	<u>US 2001-841348</u>	20010424
<u>US 6608095</u>	B2	20030819		
<u>US 2003225064</u>	A1	20031204	<u>US 2003-465767</u>	20030618
<u>US 6727238</u>	B2	20040427		
PRIORITY APPLN. INFO.:				
			<u>WO 1998-IB912</u>	W 19980611
			<u>WO 1999-IB970</u>	W 19990531
			<u>US 1999-446049</u>	A3 19991215
			<u>US 2001-841348</u>	A3 20010424

OTHER SOURCE(S): MARPAT 132:35714

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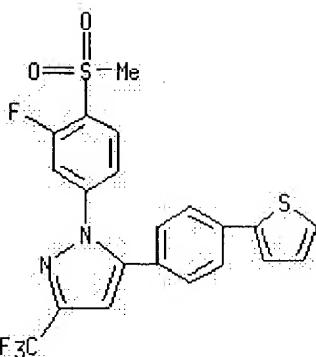
AB This invention provides a compd. of formula (I) or its pharmaceutically acceptable salt thereof [wherein A is partially unsatd. or unsatd. five membered heterocyclic, or partially unsatd. or unsatd. five membered carbocyclic, wherein the 4-(sulfonyl)phenyl and the 4-substituted Ph in formula I are attached to ring atoms of Ring A, which are adjacent to each other; R1 is optionally substituted aryl or heteroaryl, with the proviso that when A is pyrazole, R1 is heteroaryl; R2 is C1-4 alkyl, halo-substituted C1-4 alkyl, C1-4 alkylamino, C1-4 dialkylamino or amino; R3, R4 and R5 are independently hydrogen, halo, C1-4 alkyl, halo-substituted C1-4 alkyl or the like; or two of R3, R4 and R5 are taken together with atoms to which they are attached and form a 4-7 membered ring; R6 and R7 are independently hydrogen, halo, C1-4 alkyl, halo-substituted C1-4 alkyl, C1-4 alkoxy, C1-4 alkylthio, C1-4 alkylamino or N,N-di C1-4 alkylamino; and m and n are independently 1, 2, 3 or 4]. This invention also provides a pharmaceutical compn. useful for the treatment of a medical condition in which prostaglandins are implicated as pathogens. This invention relates to compd. and pharmaceutical compns. for the treatment of cyclooxygenase mediated diseases. These compds. inhibit the biosynthesis of prostaglandins by intervention of the action of the enzyme cyclooxygenase on arachidonic acid, and are therefore useful in the treatment or alleviation of inflammation and other inflammation assocd. disorders, such as arthritis, in mammals (no data). Thus, To a stirred soln. of 1-[4-(Methylsulfonyl)phenyl]-5-(4-bromophenyl)-3-trifluoromethyl-1H-pyrazole (0.27 g) in DME (8 mL) was added 3-thiophenboronic acid (0.09 g), bis(triphenylphosphine)palladium(II)chloride (0.05 g) and satd. NaHCO<sub>3</sub> soln. (2 mL) at room temp. under nitrogen. The mixt. was heated at reflux temp. for 16 h, and cooled down to room temp. to give, after purifn. by flash chromatog. eluting with Et acetate/hexane (1/1), 1-[4-(Methylsulfonyl)phenyl]-5-[4-(2-thienyl)phenyl]-3-trifluoromethyl-1H-pyrazole (II) in 64 % yield.

IT 252559-81-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of heterocycll sulfonylbenzene compds. as cyclooxygenase inhibitors, prostaglandin biosynthesis inhibitors, anti-inflammatory, and analgesic agents)

RN 252559-81-2 HCPLUS

CN 1H-Pyrazole, 1-[3-fluoro-4-(methylsulfonyl)phenyl]-5-[4-(2-thienyl)phenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 12 HCPLUS COPYRIGHT 2004 ACS on STN

Full  Abstracts  
 Text  References

ACCESSION NUMBER: 1999:82258 HCPLUS  
 DOCUMENT NUMBER: 130:210722  
 TITLE: Synthesis and properties of novel aziridinyl azo dyes from 2-aminothiophenes-Part 2: Application of some disperse dyes to polyester fibers  
 Hallas, Geoffrey; Choi, Jae-Hong  
 Dep. Colour Chemistry and Dyeing, Univ. Leeds, Leeds, LS2 9JT, UK  
 SOURCE: Dyes and Pigments (1998), Volume Date 1999, 40(2-3), 119-129  
 CODEN: DYPIDX; ISSN: 0143-7208  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A series of yellow to greenish-blue aziridinyl azo dyes and their bromoethylamino azo precursors contg. a thieryl coupling moiety has been applied to conventional polyester fiber as well as microdenier polyester by high temp. exhaust dyeing. Heat transferability of these dyes onto polyester fiber has also been examd., using conventional heat-transfer printing techniques. The relevant dyeing characteristics, heat transferability, build-up, dyeability on microfiber polyester, washfastness, and lightfastness are given. These aziridinyl dyes are reactive to polyester fibers under HT dyeing conditions. Fabrics dyed with aziridinyl dyes re more resistant to solvent extn. than those dyed with conventional dyes. Residual liquors showed only a pale color when fabric dyed with aziridinyl dyes was dissolved and then pptd., whereas a colored polyester ppt. was obtained.

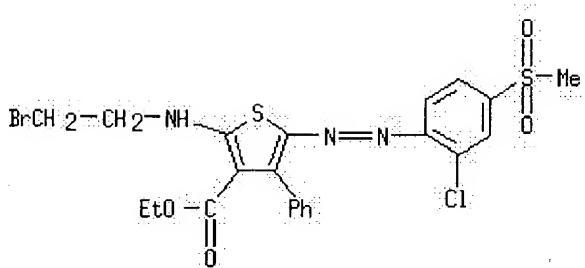
IT 220964-99-8

RL: PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(brown dye; fastness to polyester under high-temp. exhaust dyeing and thermal-transfer printing conditions)

RN 220964-99-8 HCPLUS

CN 3-Thiophenecarboxylic acid, 2-[(2-bromoethyl)amino]-5-[[2-chloro-4-(methylsulfonyl)phenyl]azo]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full Text   References

ACCESSION NUMBER: 1999:82257 HCAPLUS

DOCUMENT NUMBER: 130:210776

TITLE: Synthesis and properties of novel aziridinyl azo dyes from 2-aminothiophenes-Part 1: Synthesis and spectral properties

AUTHOR(S): Hallas, Geoffrey; Choi, Jae-Hong

CORPORATE SOURCE: Department Colour Chemistry and Dyeing, Univ. Leeds, Leeds, LS2 9JT, UK

SOURCE: Dyes and Pigments (1998), Volume Date 1999, 40(2-3), 99-117

CODEN: DYPIDX; ISSN: 0143-7208

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of yellow to greenish-blue aziridinyl azo dyes and their bromoethylamino azo precursors contg. a thieryl coupling moiety has been prepd. from 2-aminothiophenes. The 2-aminothiophenes were readily obtained by using the Gewald reaction. It was found that cyclization of the precursor dyes to the corresponding aziridine azo dyes brought about bathochromic shifts in absorption maxima. Further spectral comparisons with N-Ph azo dyes derived from other terminal 4-, 5-, 6-, 7-, and 8-membered cyclic groups showed that the N-thienylaziridinoazo dyes are relatively bathochromic. From the viewpoint of solvatochromism, a clear contrast existed between  $\lambda_{max}$  values in different solvents; thus, a pos. solvatochromism was obsd. in aprotic solvents, whereas a hypsochromic shift was brought about in polar protic solvents. PPP-MO calcns. provided reliable predictions of absorption maxima for the various aziridinyl azo dyes and their precursor dyes.

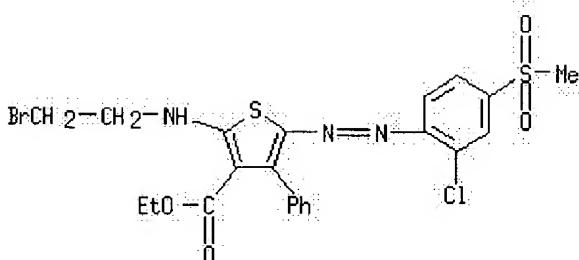
IT 220964-99-8P

RL: RCT (Reactant); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(brown dye intermediate; prepn. of aziridinyl azo dyes from 2-aminothiophene coupling components)

RN 220964-99-8 HCAPLUS

CN 3-Thiophenecarboxylic acid, 2-[(2-bromoethyl)amino]-5-[[2-chloro-4-(methylsulfonyl)phenyl]azo]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

 Full   Text  References

ACCESSION NUMBER: 1997:421308 HCAPLUS  
 DOCUMENT NUMBER: 127:34521  
 TITLE: Preparation of hydrazidyl, bis-hydrazidyl, and bis-aminomethyl carbonyl protease inhibitors  
 INVENTOR(S): Carr, Thomas Joseph; Desjarlais, Renee Louise; Gallagher, Timothy Francis; Halbert, Stacie Marie; Oh, Hye-Ja; Thompson, Scott Kevin; Veber, Daniel Frank; Yamashita, Dennis Shinji; et al.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: PCT Int. Appl., 253 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 9716433</u>	A1	19970509	<u>WO 1996-US18000</u>	19961030
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
<u>ZA 9609078</u>	A	19980429	<u>ZA 1996-9078</u>	19961029
<u>CA 2236111</u>	AA	19970509	<u>CA 1996-2236111</u>	19961030
<u>AU 9711180</u>	A1	19970522	<u>AU 1997-11180</u>	19961030
<u>CN 1207095</u>	A	19990203	<u>CN 1996-199284</u>	19961030
<u>BR 9612344</u>	A	19990713	<u>BR 1996-12344</u>	19961030
<u>EP 934291</u>	A1	19990811	<u>EP 1996-941981</u>	19961030
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO				
<u>NO 9801938</u>	A	19980629	<u>NO 1998-1938</u>	19980429
<u>US 5998470</u>	A	19991207	<u>US 1999-290958</u>	19990413
<u>US 6057362</u>	A	20000502	<u>US 1999-330287</u>	19990611
<u>US 6232342</u>	B1	20010515	<u>US 1999-330451</u>	19990611
<u>US 6284777</u>	B1	20010904	<u>US 2000-552616</u>	20000419
<u>US 6331542</u>	B1	20011218	<u>US 2000-551968</u>	20000419
<u>NO 2000006716</u>	A	19980629	<u>NO 2000-6716</u>	20001229
<u>NO 2000006717</u>	A	19980629	<u>NO 2000-6717</u>	20001229
<u>NO 2000006718</u>	A	19980629	<u>NO 2000-6718</u>	20001229
<u>CN 1341590</u>	A	20020327	<u>CN 2001-104787</u>	20010220
<u>CN 1341592</u>	A	20020327	<u>CN 2001-104788</u>	20010220

<u>CN 1341593</u>	A	20020327	<u>CN 2001-104789</u>	20010220
<u>US 2002077455</u>	A1	20020620	<u>US 2001-839410</u>	20010420
<u>US 6586466</u>	B2	20030701		
<u>US 2002173469</u>	A1	20021121	<u>US 2002-160314</u>	20020530
<u>US 6562842</u>	B2	20030513		

PRIORITY APPLN. INFO.:

<u>US 1995-8108P</u>	P	19951030
<u>US 1995-7473P</u>	P	19951122
<u>US 1995-8992P</u>	P	19951221
<u>US 1996-13747P</u>	P	19960320
<u>US 1996-13748P</u>	P	19960320
<u>US 1996-13764P</u>	P	19960320
<u>US 1996-17455P</u>	P	19960517
<u>US 1996-17892P</u>	P	19960517
<u>US 1996-22047P</u>	P	19960722
<u>US 1996-23494P</u>	P	19960807
<u>WO 1996-US18000</u>	W	19961030
<u>US 1997-793915</u>	A3	19970214
<u>US 1998-793915</u>	B3	19980430
<u>US 1999-330284</u>	B1	19990611
<u>US 1999-330305</u>	B1	19990611
<u>US 2000-633700</u>	B1	20000807

OTHER SOURCE(S):

MARPAT 127:34521

AB Title compds. of formula D-CO-Q [D = CbzNHCH(Bu-i), Cbz-Leu-NHCH(Bu-i), 4-PhOC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>NHCH<sub>2</sub>, Cbz-Leu-NHNH, etc.; Q = NHCH(Bu-i)(2-carboxythiazol-4-yl), NHCH(Bu-i)(4-carboethoxythiazol-2-yl), NHNHCOCH(Bu-i)NHCbz, CH<sub>2</sub>NHSO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>-4-OPh, etc.; Cbz = PhCH<sub>2</sub>O<sub>2</sub>C] and pharmaceutical compns. of such compds., which inhibit proteases, including cathepsin K (no data) were prep'd. Such compds. are particularly useful for treating diseases of excessive bone loss or cartilage or matrix degrdn., e.g. osteoporosis, periodontitis, and arthritis. For example, Cbz-Leu-Leu-CH<sub>2</sub>Br was treated with H<sub>2</sub>NCSCO<sub>2</sub>Et in refluxing ethanol for 4 h to give Cbz-Leu-NHCH(Bu-i)(2-carboethoxythiazol-4-yl), which was saponified by treatment with sodium hydroxide in THF to yield title compd. Cbz-Leu-NHCH(Bu-i)(2-carboxythiazol-4-yl).

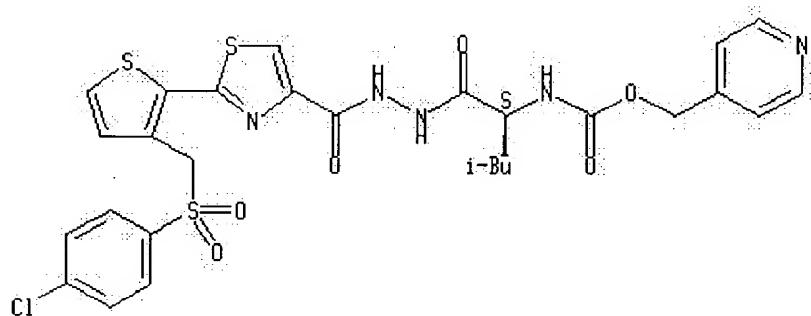
IT 190658-17-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of hydrazidyl, bis-hydrazidyl, and bis-aminomethyl carbonyl protease inhibitors)

RN 190658-17-4 HCPLUS

CN 4-Thiazolecarboxylic acid, 2-[3-[(4-chlorophenyl)sulfonyl]methyl]-2-thienyl-, 2-[(2S)-4-methyl-1-oxo-2-[(4-pyridinylmethoxy)carbonyl]amino]pentyl]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



Full Text References

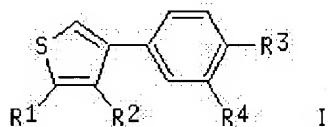
ACCESSION NUMBER: 1995:339482 HCPLUS  
 DOCUMENT NUMBER: 122:105655  
 TITLE: Preparation of 2-substituted-3,4-di(aryl)thiophene cyclooxygenase inhibitors  
 INVENTOR(S): Gauthier, Jacques Yves; Leblanc, Yves; Prasit, Petpiboon  
 PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.  
 SOURCE: PCT Int. Appl., 42 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
<u>WO 9426731</u>	A1	19941124	<u>WO 1994-CA264</u>	19940511
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, TT, UA, US, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
<u>CA 2161789</u>	AA	19941124	<u>CA 1994-2161789</u>	19940511
<u>AU 9467184</u>	A1	19941212	<u>AU 1994-67184</u>	19940511
PRIORITY APPLN. INFO.:			<u>US 1993-61354</u>	A 19930513
			<u>WO 1994-CA264</u>	W 19940511

OTHER SOURCE(S): MARPAT 122:105655

GI

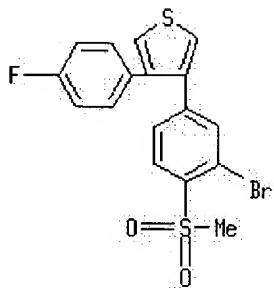


AB The title compds. [I; R1 = H, halogen, CN, NO<sub>2</sub>, CF<sub>3</sub>, C1-6 alkyl; R2 = C3-6 alkyl, (un)substituted Ph, (un)substituted heteroaryl; R3 = SO<sub>2</sub>CH<sub>3</sub>, S(O)(NH)CH<sub>3</sub>, SONH<sub>2</sub>, SO<sub>2</sub>NH<sub>2</sub>; R4 = H, halogen, CO<sub>2</sub>H, CF<sub>3</sub>], useful as cyclooxygenase inhibitors, are prep'd. and I-contg. formulations claimed. Thus, 3-(4-fluorophenyl)-4-(4-sulfamoylphenyl)thiophene was prep'd. and demonstrated 95% inhibition of PGE<sub>2</sub> formation by osteosarcoma (143.98.2) cells at 100 nM.

IT 160753-08-2

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (prep'n. of 2-substituted-3,4-di(aryl)thiophene cyclooxygenase inhibitors)

RN 160753-08-2 HCPLUSCN Thiophene, 3-[3-bromo-4-(methylsulfonyl)phenyl]-4-(4-fluorophenyl)- (9CI)  
 (CA INDEX NAME)



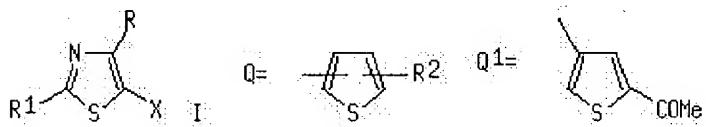
L6 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

Full  Brief  
 Text  Abstract

ACCESSION NUMBER: 1987:5016 HCAPLUS  
 DOCUMENT NUMBER: 106:5016  
 TITLE: Thiazolylthiophene derivatives  
 INVENTOR(S): Saeki, Sumi; Kawakita, Takeshi; Moriguchi, Akihiko;  
 Osuga, Kunio  
 PATENT ASSIGNEE(S): Yoshitomi Pharmaceutical Industries, Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 61118383	A2	19860605	JP 1984-237865	19841112
			JP 1984-237865	19841112
<u>PRIORITY APPLN. INFO.:</u>				
OTHER SOURCE(S):	CASREACT 106:5016			

GI



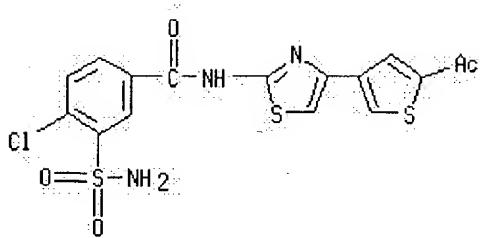
AB The title compds. [I; R = Q; R1 = (substituted) amino; R2 = alkanoyl, CH<sub>2</sub>COR<sub>3</sub> (R<sub>3</sub> = OH, alkoxy, substituted amino), X = H, halo], useful as antiulcer agents, etc. (no data), were prep'd. Thus, cyclocondensation of Q<sub>1</sub>COCH<sub>2</sub>Cl with (H<sub>2</sub>N)<sub>2</sub>CS in EtOH at 50° and acylation of the resulting I (R = Q<sub>1</sub>; R<sub>1</sub> = NH<sub>2</sub>) with pivaloyl chloride in pyridine gave I (R = Q<sub>1</sub>; R<sub>1</sub> = pivalamido).

IT 105652-30-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of, as antiulcer agent)

RN 105652-30-0 HCAPLUS

CN Benzamide, N-[4-(5-acetyl-3-thienyl)-2-thiazolyl]-3-(aminosulfonyl)-4-chloro- (9CI) (CA INDEX NAME)



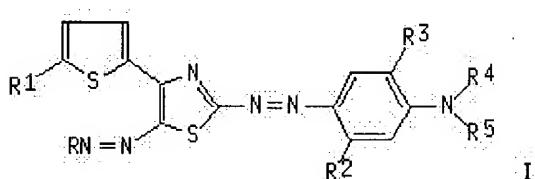
L6 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2004 ACS on STN

FULL  SEARCHED  
 Text  REFERENCES

ACCESSION NUMBER: 1983:145034 HCAPLUS  
 DOCUMENT NUMBER: 98:145034  
 TITLE: Thiénylthiazole disazo disperse dyes  
 PATENT ASSIGNEE(S): Mitsubishi Chemical Industries Co., Ltd., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 57177060	A2	19821030	JP 1981-62070	19810424
JP 01034266	B4	19890718		
GB 2101623	A	19830119	GB 1982-11221	19820419
GB 2101623	B2	19840822		
DE 3215123	A1	19821209	DE 1982-3215123	19820423
DE 3215123	C2	19900308		
CH 647537	A	19850131	CH 1982-2539	19820426
US 4841036	A	19890620	US 1984-683323	19841218
<u>PRIORITY APPLN. INFO.:</u>			JP 1981-62070	19810424
			US 1982-372264	19820426

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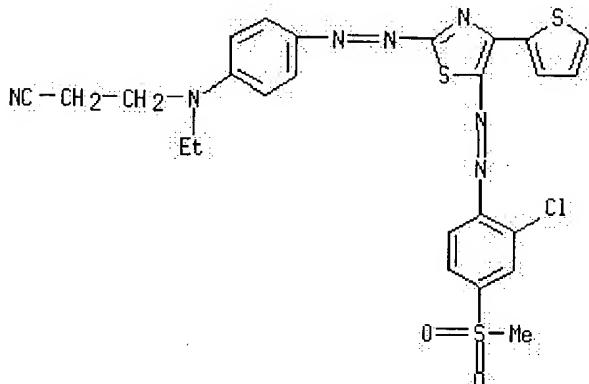
AB I (R = Ph, pyridyl, thiazolyl; R1 = H, Cl, Br, Ac; R2 = H, Cl, Br, Me, acylamino; R3 = H, Cl, Me, MeO, EtO; R4, R5 = H, alkyl, cyclohexyl, alkenyl, aryl) were prep'd. and were used for dyeing polyester fibers in fast navy blue to green shades. I showed excellent stability to temp. and pH changes during dyeing. For example, aniline [62-53-3] was diazotized and coupled with 2-amino-4-(2-thienyl)thiazole [28989-50-6], and the 2-amino-5-(phenylazo)-4-(2-thienyl)thiazole [85242-87-1] obtained was diazotized and coupled with N-(2-acetoxyethyl)-N-ethylaniline [38954-40-4] to give I (R = Ph; R1 = R2 = R3 = H; R4 = Et; R5 = CH2CH2OAc) [85242-88-2], navy blue on polyester fiber.

IT 85242-65-5

RL: TEM (Technical or engineered material use); USES (Uses)  
 (dye, for polyester fibers)

RN 85242-65-5 HCAPLUS

CN Propanenitrile, 3-[[4-[[5-[[2-chloro-4-(methylsulfonyl)phenyl]azo]-4-(2-thienyl)-2-thiazolyl]azo]phenyl]ethylamino]- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS

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ENTRY

SESSION

FULL ESTIMATED COST

74.92

231.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

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L3 41 S L1 FULL

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L4 14 S L3

L5 2 S L4 AND BROWN, D?/AU

L6 12 S L4 NOT L5  
L7 0 S L6 AND GRANETO, M?/AU  
L8 0 S L6 AND LUDWIG, C?/AU

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